1. SUPPLEMENTAL MATERIAL

- Cut off parameters in fragments analysis using "BondFrag" code

Bond	Cut off
C-N	0.30
C-C	0.55
C-O	0.80
C-H	0.40
O-O	0.65
N-O	0.55
O-H	0.40
H-H	0.55
H-N	0.55
N-N	0.55

- Potential parameters used in ReaxFF

Reactive MD-force field: nitramines (RDX/HMX /TATB/PETN)+DMNA-barrier+innervdWaa
39 ! Number of general parameters
50.0000 !Overcoordination parameter
9.4514 !Overcoordination parameter
29.8953 !Valency angle conjugation parameter
216.5421 !Triple bond stabilisation parameter
12.2245 !Triple bond stabilisation parameter
0.0000 !C2-correction
1.0701 !Undercoordination parameter
7.5000 !Triple bond stabilisation parameter
11.9083 !Undercoordination parameter
13.3822 !Undercoordination parameter
-10.9834 !Triple bond stabilization energy
0.0000 !Lower Taper-radius
10.0000 !Upper Taper-radius
2.8793 !Not used
33.8667 !Valency undercoordination
3.3976 !Valency angle/lone pair parameter
1.0563 !Valency angle
2.0384 !Valency angle parameter
6.1431 !Not used
6.9290 !Double bond/angle parameter
0.0283 !Double bond/angle parameter: overcoord
0.0570 !Double bond/angle parameter: overcoord
-2.4837 !Not used
5.8374 !Torsion/BO parameter
10.0000 !Torsion overcoordination
1.8820 !Torsion overcoordination
-1.2327 !Conjugation 0 (not used)
2.1861 !Conjugation

1.5591 !vdWaals shielding
0.0100 !Cutoff for bond order (*100)
4.8414 !Valency angle conjugation parameter
3.5857 !Overcoordination parameter
38.6472 !Overcoordination parameter
2.1533 !Valency/lone pair parameter
0.5000 !Not used
20.0000 !Not used
5.0000 !Molecular energy (not used)
0.0000 !Molecular energy (not used)
6.9784 !Valency angle conjugation parameter
7 !Nr of atoms;cov.r;

valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#alfa;gammavdW;valency;Eunder;Eover;chiEEM;
etaEEM;n.u.;cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.;ov/un;val1;n.u.;val3,vval4
C 1.3742 4.0000 12.0000 1.9684 0.1723 0.8712 1.2385 4.0000
8.7696 100.0000 4.0000 31.0823 79.5548 5.7254 6.9235 0.0000
1.2104 0.0000 183.8108 5.7419 33.3951 11.9957 0.8563 0.0000
-2.8983 4.7820 1.0564 4.0000 2.9663 1.6737 0.1421 14.0707
H 0.6867 1.0000 1.0080 1.3525 0.0616 0.8910 -0.1000 1.0000
9.1506 100.0000 1.0000 0.0000 121.1250 3.8446 10.0839 1.0000
-0.1000 0.0000 58.4369 3.8461 3.2540 1.0000 1.0698 0.0000
-15.7683 2.1504 1.0338 1.0000 2.8793 1.2669 0.0139 12.4538
O 1.3142 2.0000 15.9990 1.9741 0.0880 0.8712 1.1139 6.0000
9.9926 100.0000 4.0000 29.5271 116.0768 8.5000 7.1412 2.0000
0.9909 14.7235 69.2921 9.1371 1.6258 0.1863 0.9745 0.0000
-3.5965 2.5000 1.0493 4.0000 2.9225 1.7221 0.1670 13.9991
N 1.2456 3.0000 14.0000 2.0437 0.1035 0.8712 1.1911 5.0000
9.8823 100.0000 4.0000 32.4758 100.0000 6.8453 6.8349 2.0000
1.0636 0.0276 127.9672 2.2169 2.8632 2.4419 0.9745 0.0000
-4.0959 2.0047 1.0183 4.0000 2.8793 1.5967 0.1649 13.9888
S 1.9647 2.0000 32.0600 2.0783 0.2176 1.0336 1.5386 6.0000
9.9676 5.0812 4.0000 35.1648 112.1416 6.5000 8.2545 2.0000
1.4703 9.4922 70.0338 8.5146 28.0801 8.5010 0.9745 0.0000
-10.0773 2.7466 1.0338 6.2998 2.8793 1.8000 0.0000 14.0000
Si 2.0276 4.0000 28.0600 2.2042 0.1322 0.8218 1.5758 4.0000
11.9413 2.0618 4.0000 11.8211 136.4845 1.8038 7.3852 0.0000
-1.0000 0.0000 126.5331 6.4918 8.5961 0.2368 0.8563 0.0000
-3.8112 3.1873 1.0338 4.0000 2.5791 0.0000 0.0000 0.0000
X -0.1000 2.0000 1.0080 2.0000 0.0000 1.0000 -0.1000 6.0000
10.0000 2.5000 4.0000 0.0000 0.0000 8.5000 1.5000 0.0000
-0.1000 0.0000 -2.3700 8.7410 13.3640 0.6690 0.9745 0.0000
-11.0000 2.7466 1.0338 4.0000 2.8793 0.0000 0.0000 0.0000
18 !Nr of bonds;Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6;pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;
ovcorr
1 1 141.9346 113.4487 67.6027 0.1554 -0.3045 1.0000 30.4515 0.4283

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      0.0801  -0.2113   8.5395   1.0000  -0.0933   6.6967   1.0000   0.0000
 1  2 163.6889   0.0000   0.0000  -0.4525   0.0000   1.0000   6.0000   0.5921
     12.1053   1.0000   0.0000   1.0000  -0.0097   8.6351   0.0000   0.0000
 2  2 169.8421   0.0000   0.0000  -0.3591   0.0000   1.0000   6.0000   0.7503
      9.3119   1.0000   0.0000   1.0000  -0.0169   5.9406   0.0000   0.0000
 1  3 159.7219 116.8921  77.9315  -0.4324  -0.1742   1.0000  15.0019   0.5160
      1.2934  -0.3079   7.0252   1.0000  -0.1543   4.5116   0.0000   0.0000
 3  3 108.9631 158.3501  42.0558   0.1226  -0.1324   1.0000  28.5716   0.2545
      1.0000  -0.2656   8.6489   1.0000  -0.1000   6.8482   1.0000   0.0000
 1  4 128.9104 171.2945 100.5836  -0.1306  -0.4948   1.0000  26.7458   0.4489
      0.3746  -0.3549   7.0000   1.0000  -0.1248   4.9232   1.0000   0.0000
 3  4  85.0402 118.8680  75.7263   0.7080  -0.1062   1.0000  16.6913   0.2407
      0.3535  -0.1906   8.4054   1.0000  -0.1154   5.6575   1.0000   0.0000
 4  4 160.6599  73.3721 154.2849  -0.7107  -0.1462 1.0000  12.0000   0.6826
      0.9330  -0.1434  10.6712   1.0000  -0.0890   4.6486   1.0000   0.0000
 2  3 219.7016   0.0000   0.0000  -0.6643   0.0000   1.0000   6.0000   0.9854
      5.1146   1.0000   0.0000   1.0000  -0.0532   5.1189   0.0000   0.0000
 2  4 208.0443   0.0000   0.0000  -0.3923   0.0000   1.0000   6.0000   0.3221
     10.5505   1.0000   0.0000   1.0000  -0.0690   6.2949   0.0000   0.0000
 1  5 128.7959  56.4134  39.0716   0.0688  -0.4463   1.0000  31.1766   0.4530
      0.1955  -0.3587   6.2148   1.0000  -0.0770   6.6386   1.0000   0.0000
 2  5 128.6090   0.0000   0.0000  -0.5555   0.0000   1.0000   6.0000   0.4721
     10.8735   1.0000   0.0000   1.0000  -0.0242   9.1937   1.0000   0.0000
 3  5   0.0000   0.0000   0.0000   0.5563  -0.4038   1.0000  49.5611   0.6000
      0.4259  -0.4577  12.7569   1.0000  -0.1100   7.1145   1.0000   0.0000
 4  5   0.0000   0.0000   0.0000   0.4438  -0.2034   1.0000  40.3399   0.6000
      0.3296  -0.3153   9.1227   1.0000  -0.1805   5.6864   1.0000   0.0000
 5  5  96.1871  93.7006  68.6860   0.0955  -0.4781   1.0000  17.8574   0.6000
      0.2723  -0.2373   9.7875   1.0000  -0.0950   6.4757   1.0000   0.0000
 6  6 109.1904  70.8314  30.0000   0.2765  -0.3000   1.0000  16.0000   0.1583
      0.2804  -0.1994   8.1117   1.0000  -0.0675   8.2993   0.0000   0.0000
 2  6 137.1002   0.0000   0.0000  -0.1902   0.0000   1.0000   6.0000   0.4256
     17.7186   1.0000   0.0000   1.0000  -0.0377   6.4281   0.0000   0.0000
 3  6 191.1743  52.0733  43.3991  -0.2584  -0.3000   1.0000  36.0000   0.8764
      1.0248  -0.3658   4.2151   1.0000  -0.5004   4.2605   1.0000   0.0000
10    ! Nr of off-diagonal terms;Ediss;Ro;gamma;rsigma; rpi;rpi2
 1  2   0.0464   1.8296   9.9214   1.0029  -1.0000  -1.0000
 2  3   0.0403   1.6913  10.4801   0.8774  -1.0000  -1.0000
 2  4   0.0524   1.7325  10.1306   0.9982  -1.0000  -1.0000
 1  3   0.1028   1.9277   9.1521   1.3399   1.1104   1.1609
 1  4   0.2070   1.7366   9.5916   1.2960   1.2008   1.1262
 3  4   0.0491   1.7025  10.6101   1.3036   1.1276   1.0173
 2  6   0.0470   1.6738  11.6877   1.1931  -1.0000  -1.0000
 3  6   0.1263   1.8163  10.6833   1.6266   1.2052  -1.0000
 1  5   0.1408   1.8161   9.9393   1.7986   1.3021   1.4031
 2  5   0.0895   1.6239  10.0104   1.4640  -1.0000  -1.0000
```

62 ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
1 1 1 74.0317 32.2712 0.9501 0.0000 0.1780 10.5736 1.0400
1 1 2 70.6558 14.3658 5.3224 0.0000 0.0058 0.0000 1.0400
2 1 2 76.7339 14.4217 3.3631 0.0000 0.0127 0.0000 1.0400
1 2 2 0.0000 0.0000 6.0000 0.0000 0.0000 0.0000 1.0400
1 2 1 0.0000 3.4110 7.7350 0.0000 0.0000 0.0000 1.0400
2 2 2 0.0000 27.9213 5.8635 0.0000 0.0000 0.0000 1.0400
1 1 3 65.1700 8.0170 7.5000 0.0000 0.2028 10.0000 1.0400
3 1 3 71.7582 26.7070 6.0466 0.0000 0.2000 0.0000 1.8525
1 1 4 65.4228 43.9870 1.5602 0.0000 0.2000 10.0000 1.8525
3 1 4 73.7046 23.8131 3.9811 0.0000 0.2000 0.0000 1.8525
4 1 4 65.6602 40.5852 1.8122 0.0000 0.2000 0.0000 1.8525
2 1 3 56.4426 17.6020 5.3044 0.0000 0.9699 0.0000 1.1272
2 1 4 71.0777 9.1462 3.4142 0.0000 0.9110 0.0000 1.0400
1 2 4 0.0000 0.0019 6.3000 0.0000 0.0000 0.0000 1.0400
1 3 1 72.1018 38.4720 1.3926 0.0000 0.4785 0.0000 1.2984
1 3 3 89.9987 44.9806 0.5818 0.0000 0.7472 0.0000 1.2639
1 3 4 70.3281 12.9371 7.5000 0.0000 0.7472 0.0000 1.2639
3 3 3 84.2807 24.1938 2.1695 -10.0000 0.7472 0.0000 1.2639
3 3 4 84.2585 44.1039 0.9185 0.0000 0.7472 0.0000 1.2639
4 3 4 74.2312 25.7005 4.3943 0.0000 0.7472 0.0000 1.2639
1 3 2 89.0416 36.9460 0.4569 0.0000 2.7636 0.0000 2.0494
2 3 3 81.1709 4.2886 6.5904 0.0000 3.0000 0.0000 1.2618
2 3 4 75.9203 44.9675 0.8889 0.0000 3.0000 0.0000 1.2618
2 3 2 82.2020 12.7165 3.9296 0.0000 0.2765 0.0000 1.0470
1 4 1 68.3788 18.3716 1.8893 0.0000 2.4132 0.0000 1.3993
1 4 3 86.5585 37.6814 1.1611 0.0000 1.7325 0.0000 1.0440
1 4 4 74.4818 12.0954 7.5000 0.0000 1.7325 0.0000 1.0440
3 4 3 78.5850 44.3389 1.3239 -26.2246 1.7325 40.0000 1.0440
3 4 4 77.6245 32.0866 1.8889 -0.9193 1.7325 0.0000 1.0440
4 4 4 66.4718 15.9087 7.5000 0.0000 1.7325 0.0000 1.0440
1 4 2 90.0000 33.6636 1.1051 0.0000 0.2638 0.0000 1.1376
2 4 3 83.8493 44.9000 1.3580 0.0000 0.5355 0.0000 2.5279
2 4 4 78.7452 24.2010 3.7481 0.0000 0.5355 0.0000 2.5279
2 4 2 55.8679 14.2331 2.9225 0.0000 0.2000 0.0000 2.9932
1 2 3 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
1 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
1 2 5 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
3 2 3 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
3 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
4 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
2 2 3 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
2 2 4 0.0000 0.0019 6.0000 0.0000 0.0000 0.0000 1.0400
1 1 5 74.4180 33.4273 1.7018 0.1463 0.5000 0.0000 1.6178
1 5 1 79.7037 28.2036 1.7073 0.1463 0.5000 0.0000 1.6453
2 1 5 63.3289 29.4225 2.1326 0.0000 0.5000 0.0000 3.0000

```
 1  5  2  85.9449  38.3109   1.2492   0.0000   0.5000   0.0000   1.1000
 1  5  5  85.6645  40.0000   2.9274   0.1463   0.5000   0.0000   1.3830
 2  5  2  83.8555   5.1317   0.4377   0.0000   0.5000   0.0000   3.0000
 2  5  5  97.0064  32.1121   2.0242   0.0000   0.5000   0.0000   2.8568
 6  6  6  69.3456  21.7361   1.4283   0.0000  -0.2101   0.0000   1.3241
 2  6  6  75.6168  21.5317   1.0435   0.0000   2.5179   0.0000   1.0400
 2  6  2  78.3939  20.9772   0.8630   0.0000   2.8421   0.0000   1.0400
 3  6  6  70.3016  15.4081   1.3267   0.0000   2.1459   0.0000   1.0400
 2  6  3  73.8232  16.6592   3.7425   0.0000   0.8613   0.0000   1.0400
 3  6  3  90.0344   7.7656   1.7264   0.0000   0.7689   0.0000   1.0400
 6  3  6  22.1715   3.6615   0.3160   0.0000   4.1125   0.0000   1.0400
 2  3  6  83.7634   5.6693   2.7780   0.0000   1.6982   0.0000   1.0400
 3  3  6  73.4663  25.0761   0.9143   0.0000   2.2466   0.0000   1.0400
 2  2  6   0.0000  47.1300   6.0000   0.0000   1.6371   0.0000   1.0400
 6  2  6   0.0000  31.5209   6.0000   0.0000   1.6371   0.0000   1.0400
 3  2  6   0.0000  31.0427   4.5625   0.0000   1.6371   0.0000   1.0400
 2  2  5   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
31 ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO); vconj;n.u;n
 1  1  1  1   0.0000  48.4194   0.3163  -8.6506  -1.7255   0.0000   0.0000
 1  1  1  2   0.0000  63.3484   0.2210  -8.8401  -1.8081   0.0000   0.0000
 2  1  1  2   0.0000  45.2741   0.4171  -6.9800  -1.2359   0.0000   0.0000
 0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  1  3  0   1.7254  86.0769   0.3440  -4.2330  -2.0000   0.0000   0.0000
 0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  3  0   1.2314 116.5137   0.5599  -4.1412   0.0000   0.0000   0.0000
 0  1  4  0  -1.3258 149.8644   0.4790  -7.1541  -2.0000   0.0000   0.0000
 0  2  4  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  4  0   1.3168  57.0732   0.2679  -4.1516  -2.0000   0.0000   0.0000
 0  4  4  0   2.0000  75.3685  -0.7852  -9.0000  -2.0000   0.0000   0.0000
 0  1  1  0   0.0930  18.6070  -1.3191  -9.0000  -1.0000   0.0000   0.0000
 4  1  4  4  -2.0000  20.6655  -1.5000  -9.0000  -2.0000   0.0000   0.0000
 0  1  5  0   4.0885  78.7058   0.1174  -2.1639   0.0000   0.0000   0.0000
 0  5  5  0  -0.0170 -56.0786   0.6132  -2.2092   0.0000   0.0000   0.0000
 0  2  5  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  6  6  0   0.0000   0.0000   0.1200  -2.4426   0.0000   0.0000   0.0000
 0  2  6  0   0.0000   0.0000   0.1200  -2.4847   0.0000   0.0000   0.0000
 0  3  6  0   0.0000   0.0000   0.1200  -2.4703   0.0000   0.0000   0.0000
 1  1  3  3   1.2707  21.6200   1.5000  -9.0000  -2.0000   0.0000   0.0000
 1  3  3  1  -1.8804  79.9255  -1.5000  -4.1940  -2.0000   0.0000   0.0000
 3  1  3  3  -2.0000  22.5092   1.5000  -8.9500  -2.0000   0.0000   0.0000
 1  4  4  3   0.1040  70.1152   0.5284  -3.5026  -2.0000   0.0000   0.0000
 1  1  3  4   1.2181 119.6186  -1.5000  -7.0635  -2.0000   0.0000   0.0000
 2  1  3  4  -2.0000 156.6604   1.1004  -7.3729  -2.0000   0.0000   0.0000
 1  3  4  3   2.0000  96.6281  -1.5000  -3.8076  -2.0000   0.0000   0.0000
 1  1  4  2  -2.0000 147.2445  -1.5000  -7.0142  -2.0000   0.0000   0.0000
```

1 1 4 3 -2.0000 47.8326 -1.5000 -9.0000 -2.0000 0.0000 0.0000
2 3 4 3 -0.2997 152.9040 -1.5000 -4.4564 -2.0000 0.0000 0.0000
2 4 4 3 0.1040 70.1152 0.5284 -3.5026 -2.0000 0.0000 0.0000
9 ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
3 2 3 2.1845 -2.3549 3.0582 19.1627
3 2 4 1.6658 -3.8907 3.0582 19.1627
4 2 3 1.8738 -3.5421 3.0582 19.1627
4 2 4 1.8075 -4.1846 3.0582 19.1627
3 2 5 2.6644 -3.0000 3.0000 3.0000
4 2 5 4.0476 -3.0000 3.0000 3.0000
5 2 3 2.1126 -4.5790 3.0000 3.0000
5 2 4 2.2066 -5.7038 3.0000 3.0000
5 2 5 1.9461 -4.0000 3.0000 3.0000